**Table S1. Differentiating metabolites between the control (C\_BW) and moderate concentration BDE-47 treatment (M\_BW) groups (*P* < 0.01).**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Metabolite** | **Mass (Da)** | **Formula** | **Mode** | **Regulate** | ***P*** | **FDR** |
| (S)-10,16-Dihydroxyhexadecanoic acid | 306.2632 | C16H32O4 | pos | up | 0.003508 | 0.0894 |
| Epigallocatechin gallate | 441.0815 | C22H18O11 | pos | down | 0.000011 | 0.0026 |
| Ascorbyl stearate | 460.3264 | C24H42O7 | pos | down | 0.001300 | 0.0487 |
| 8(R)-HETE | 303.2312 | C20H32O3 | pos | up | 0.004984 | 0.1126 |
| PC(16:0/0:0) | 518.3213 | C24H50NO7P | pos | up | 0.003515 | 0.0894 |
| Gallic acid | 171.0281 | C7H6O5 | pos | down | 0.000139 | 0.0101 |
| PC(17:0/0:0) | 510.3553 | C25H52NO7P | pos | up | 0.001503 | 0.0518 |
| 9,12,15-hexadecatrienoic acid | 251.1998 | C16H26O2 | pos | up | 0.005256 | 0.1145 |
| 24-Nor-5beta-cholane-3alpha,7alpha,12alpha,22,23-pentol | 397.2944 | C23H40O5 | pos | down | 0.007970 | 0.1315 |
| PE(22:6/0:0) | 526.2934 | C27H44NO7P | pos | up | 0.007768 | 0.1310 |
| 3-hydroxyundecanoyl carnitine | 310.2352 | C18H35NO5 | pos | down | 0.007063 | 0.1278 |
| Elaidamide | 282.2783 | C18H35NO | pos | down | 0.000877 | 0.0364 |
| Avocadene | 304.2831 | C17H34O3 | pos | up | 0.003426 | 0.0890 |
| 16-Hydroxy hexadecanoic acid | 290.2681 | C16H32O3 | pos | up | 0.005964 | 0.1192 |
| Myristic acid | 246.2420 | C14H28O2 | pos | up | 0.006201 | 0.1214 |
| Hydroxynalidixic acid | 271.0705 | C12H12N2O4 | pos | down | 0.001262 | 0.0477 |
| 2-trans,4-cis-Decadienoylcarnitine | 344.2429 | C17H29NO4 | pos | up | 0.009313 | 0.1411 |
| 9,10,13-Trihydroxystearic acid | 350.2900 | C18H36O5 | pos | up | 0.002882 | 0.0803 |
| Ethyl 3-hydroxydodecanoate | 262.2369 | C14H28O3 | pos | up | 0.002106 | 0.0638 |
| Guanosine triphosphate adenosine | 737.0640 | C20H27N10O17P3 | pos | down | 0.006178 | 0.1214 |
| Astragalin | 449.1075 | C21H20O11 | pos | down | 0.000004 | 0.0018 |
| 2-(2,4,5-trihydroxyphenyl)propanoic acid | 199.0591 | C9H10O5 | pos | down | 0.000018 | 0.0029 |
| Argininosuccinic acid | 273.1219 | C10H18N4O6 | pos | up | 0.000554 | 0.0264 |
| Aminocaproic acid | 132.1015 | C6H13NO2 | pos | up | 0.000109 | 0.0085 |
| Lysinoalanine | 198.1228 | C9H19N3O4 | pos | up | 0.009915 | 0.1460 |
| Ethyl 2-mercaptopropionate | 135.0469 | C5H10O2S | pos | up | 0.006949 | 0.1269 |
| Inosine | 267.0721 | C10H12N4O5 | neg | up | 0.001764 | 0.0675 |
| LysoPC(0:0/16:0) | 540.3268 | C24H50NO7P | neg | up | 0.001614 | 0.0668 |
| Glycitein 7-O-glucuronide | 459.0910 | C22H20O11 | neg | down | 0.000564 | 0.0440 |
| MG(i-17:0/0:0/0:0) | 389.2904 | C20H40O4 | neg | down | 0.000360 | 0.0338 |
| Polyoxyethylene 40 monostearate | 373.2943 | C20H40O3 | neg | down | 0.001264 | 0.0593 |
| Oxmetidine | 420.1139 | C19H21N5O3S | neg | up | 0.005858 | 0.1123 |
| Docosapentaenoic acid (22n-6) | 375.2521 | C22H34O2 | neg | up | 0.006340 | 0.1167 |
| MG(18:0/0:0/0:0) | 403.3050 | C21H42O4 | neg | down | 0.000260 | 0.0322 |
| Ethotoin | 239.0589 | C11H12N2O2 | neg | down | 0.000350 | 0.0338 |
| 5-(3',4',5'-trihydroxyphenyl)-gamma-valerolactone-O-methyl-4'-O-glucuronide | 435.0950 | C18H22O11 | neg | up | 0.009529 | 0.1425 |
| Quercitrin | 447.0937 | C21H20O11 | neg | down | 0.005149 | 0.1060 |
| Quercetin 3-beta-D-glucoside | 463.0884 | C21H20O12 | neg | down | 0.000221 | 0.0286 |
| Adenosine | 312.0934 | C10H13N5O4 | neg | down | 0.007250 | 0.1241 |
| Fagomine | 184.0373 | C6H13NO3 | neg | up | 0.009639 | 0.1434 |
| 3-Hexenedioic acid | 125.0242 | C6H8O4 | neg | down | 0.000468 | 0.0399 |
| 4-Nitrophenol | 138.0191 | C6H5NO3 | neg | up | 0.002500 | 0.0740 |

**Table S2. Differentiating metabolites between the control (C\_BW) and high concentration BDE-47 treatment (H\_BW) groups (*P* < 0.01).**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Metabolite** | **Mass (Da)** | **Formula** | **Mode** | **Regulate** | ***P*** | **FDR** |
| Aphidicolin | 361.2232 | C20H34O4 | pos | down | 0.00263 | 0.0780 |
| LysoPC(P-16:0) | 480.3422 | C24H50NO6P | pos | down | 0.002249 | 0.0704 |
| Cis-3-Hexenyl phenylacetate | 236.1637 | C14H18O2 | pos | up | 0.002608 | 0.0780 |
| 2-(8-[3]-ladderane-octanyl)-sn-glycero-3-phosphoethanolamine | 488.3105 | C25H46NO6P | pos | down | 0.000660 | 0.0300 |
| Osmundalactone | 111.0440 | C6H8O3 | pos | up | 0.004352 | 0.1065 |
| 16beta-16-Hydroxy-3-oxo-1,12-oleanadien-28-oic acid | 469.3308 | C30H44O4 | pos | up | 0.007860 | 0.1546 |
| Normeperidinic acid | 206.1183 | C12H15NO2 | pos | up | 0.007983 | 0.1562 |
| 1400W | 178.1330 | C10H15N3 | pos | up | 0.002727 | 0.0783 |
| 2-Pentyl-3-phenyl-2-propenal | 443.2324 | C14H18O | pos | down | 0.006701 | 0.1399 |
| Melleolide B | 474.2480 | C24H32O7 | pos | down | 0.002705 | 0.0783 |
| Epigallocatechin gallate | 441.0815 | C22H18O11 | pos | down | 0.000008 | 0.0013 |
| 1-hexadecyl-glycero-3-phosphate | 438.2969 | C19H41O6P | pos | down | 0.002970 | 0.0840 |
| LysoPE(20:0/0:0) | 492.3441 | C25H52NO7P | pos | down | 0.000768 | 0.0331 |
| LysoPC(20:5(5Z,8Z,11Z,14Z,17Z)) | 524.3090 | C28H48NO7P | pos | down | 0.006819 | 0.1406 |
| Gallic acid | 171.0281 | C7H6O5 | pos | down | 0.000259 | 0.0152 |
| PE(20:5/0:0) | 522.2588 | C25H42NO7P | pos | down | 0.001759 | 0.0611 |
| Avenestergenin A2 | 650.4108 | C37H52O7 | pos | up | 0.005471 | 0.1261 |
| Asparagoside C | 763.4263 | C39H64O13 | pos | up | 0.002864 | 0.0816 |
| 2,3,23-Triacetylsericic acid | 631.3840 | C36H54O9 | pos | up | 0.007725 | 0.1528 |
| 6-{[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]methyl}oxane-2,3,4,5-tetrol | 309.1167 | C12H22O10 | pos | up | 0.004082 | 0.1018 |
| Hydroxynalidixic acid | 271.0705 | C12H12N2O4 | pos | down | 0.000037 | 0.0040 |
| Astragalin | 449.1075 | C21H20O11 | pos | down | 0.000060 | 0.0051 |
| Vidarabine | 268.1033 | C10H13N5O4 | pos | down | 0.000176 | 0.0110 |
| 2-(2,4,5-trihydroxyphenyl)propanoic acid | 199.0591 | C9H10O5 | pos | down | 0.000004 | 0.0009 |
| Calcitroic acid | 395.2181 | C23H34O4 | neg | down | 0.000093 | 0.0198 |
| 2-cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-diethylpropanamide | 342.0849 | C14H17N3O5 | neg | up | 0.003462 | 0.1185 |
| Leukotriene D5 | 531.1942 | C25H38N2O6S | neg | down | 0.007790 | 0.1710 |
| Glycitein 7-O-glucuronide | 459.0910 | C22H20O11 | neg | down | 0.000358 | 0.0395 |
| Suillusin | 415.0649 | C19H14O8 | neg | down | 0.003962 | 0.1226 |
| MG(i-17:0/0:0/0:0) | 389.2904 | C20H40O4 | neg | down | 0.000137 | 0.0265 |
| Polyoxyethylene 40 monostearate | 373.2943 | C20H40O3 | neg | down | 0.004357 | 0.1262 |
| MG(19:0/0:0/0:0) | 393.2992 | C22H44O4 | neg | down | 0.003826 | 0.1222 |
| Tragopogonsaponin A | 669.3678 | C36H56O10 | neg | up | 0.003836 | 0.1222 |
| (4E,7E,10Z,13E,16E,19E)-docosa-4,7,10,13,16,19-hexaenoic acid | 327.2310 | C22H32O2 | neg | down | 0.000179 | 0.0299 |
| PE(21:0/0:0) | 522.3545 | C26H54NO7P | neg | down | 0.009982 | 0.1900 |
| (3b,4b,11b,14b)-11-Ethoxy-3,4-epoxy-14-hydroxy-12-cyathen-15-al 14-xyloside | 529.2607 | C27H42O8 | neg | down | 0.000616 | 0.0508 |
| Protoporphyrinogen IX | 589.2797 | C34H40N4O4 | neg | up | 0.008269 | 0.1772 |
| PE(22:0/0:0) | 536.3708 | C27H56NO7P | neg | down | 0.004163 | 0.1256 |
| (-)-Stercobilin | 631.2957 | C33H46N4O6 | neg | down | 0.002028 | 0.0952 |
| Avenestergenin B2 | 573.3625 | C37H52O6 | neg | up | 0.008724 | 0.1827 |
| 3-trans-Caffeoyltormentic acid | 631.3659 | C39H54O8 | neg | up | 0.004197 | 0.1256 |
| Quercetin 3-beta-D-glucoside | 463.0884 | C21H20O12 | neg | down | 0.003706 | 0.1215 |
| Adenosine | 312.0934 | C10H13N5O4 | neg | down | 0.000075 | 0.0198 |
| 3-Hexenedioic acid | 125.0242 | C6H8O4 | neg | down | 0.000373 | 0.0395 |

**Table S3. Differentiating metabolites shared in the low and moderate-concentration groups (*p* < 0.05)**

|  |  |  |
| --- | --- | --- |
| **Metabolite** | **FC** | ***p* value** |
| **Low/Control** | **Moderate/Control** | **Low** | **Moderate** |
| Thiamine monophosphate | 1.3765 | 1.3688 | 0.032100 | 0.030680 |
| 9,10,13-Trihydroxystearic acid | 1.1432 | 1.2151 | 0.024930 | 0.002882 |
| Sphinganine | 1.0378 | 1.0388 | 0.008008 | 0.017220 |
| Avocadene | 1.1160 | 1.1462 | 0.005559 | 0.003426 |
| 16-Hydroxy hexadecanoic acid | 1.0352 | 1.0560 | 0.009172 | 0.005964 |
| C16 Sphinganine | 1.0272 | 1.0322 | 0.003494 | 0.011850 |
| L-3,5-Diiodotyrosine | 1.2140 | 1.2092 | 0.000718 | 0.011770 |
| Ethyl 3-hydroxydodecanoate | 1.0715 | 1.0987 | 0.003099 | 0.002106 |
| Myristic acid | 1.0427 | 1.0683 | 0.010080 | 0.006201 |
| Xestoaminol C | 1.0258 | 1.0309 | 0.022740 | 0.034730 |
| (4-{2-[(1R,16Z,24Z,29Z)-1,18-dihydroxy-19,31-dimethoxy-15,17,21,23,30,36-hexamethyl-2,3,10,14,20-pentaoxo-11,27,37-trioxa-4-azatetracyclo[31.3.1.0?,?.0??,??]heptatriaconta-16,24,29-trien-12-yl]propyl}-2-methoxycyclohexyl)oxidanesulfonic acid | 1.7600 | 2.1992 | 0.014650 | 0.000017 |
| (S)-10,16-Dihydroxyhexadecanoic acid | 1.0311 | 1.0461 | 0.007156 | 0.003508 |
| 2-Ethyl-1-hexanol sulfate | 1.1069 | 1.1232 | 0.043630 | 0.021140 |
| 1-Acetoxy-2-hydroxy-16-heptadecyn-4-one | 0.8700 | 1.1804 | 0.031630 | 0.014680 |
| 3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid | 0.8143 | 1.0860 | 0.003208 | 0.011260 |
| Fagomine | 0.9068 | 1.0710 | 0.040070 | 0.009639 |
| Citric acid | 0.7246 | 1.2500 | 0.019430 | 0.042030 |
| Inosine | 0.9469 | 1.0284 | 0.004212 | 0.001764 |
| S-(11-hydroxy-9-deoxy-delta12-PGD2)-glutathione | 0.2696 | 0.2113 | 0.031950 | 0.021620 |
| Persenone B | 0.4107 | 0.5858 | 0.001179 | 0.018480 |

**Table S4. Differentiating metabolites shared in the low and high-concentration groups**

**(*p* < 0.05)**

|  |  |  |
| --- | --- | --- |
| **Metabolite** | **FC** | ***p value*** |
| **Low/Control** | **High/Control** | **Low** | **High** |
| DG(18:1(9Z)/18:2(9Z,12Z)/0:0)[iso2] | 0.7710 | 0.7276 | 0.029330 | 0.019880 |
| Ikshusterol | 0.9187 | 0.8835 | 0.045850 | 0.012450 |
| (4E,7E,10Z,13E,16E,19E)-docosa-4,7,10,13,16,19-hexaenoic acid | 0.9772 | 0.9662 | 0.018650 | 0.000179 |
| MG(19:0/0:0/0:0) | 0.7120 | 0.3153 | 0.008022 | 0.003826 |
| 2-Pentyl-3-phenyl-2-propenal | 0.7907 | 0.7677 | 0.005829 | 0.006701 |
| 16(R)-HETE | 0.9265 | 0.9522 | 0.046880 | 0.032390 |
| Normeperidinic acid | 0.8889 | 1.1409 | 0.009752 | 0.007983 |
| L-Phenylalanine n-butyl ester | 0.8188 | 1.1255 | 0.012980 | 0.023070 |
| Leu Lys Ala Val Val | 0.8747 | 1.0991 | 0.040870 | 0.038720 |
| Avenestergenin B2 | 0.8786 | 1.0673 | 0.046030 | 0.008724 |
| Lyciumoside VIII | 0.5489 | 1.4350 | 0.011830 | 0.033660 |

**Table S5. Differentiating metabolites shared in the moderate and high-concentration groups**

 **(*p* < 0.05)**

|  |  |  |
| --- | --- | --- |
| **Metabolite** | **FC** | ***p value*** |
| **Moderate/Control** | **High/Control** | **Moderate** | **High** |
| Molybdopterin precursor Z | 0.6270 | 0.5846 | 0.017160 | 0.047950 |
| Ethotoin | 0.8969 | 0.8850 | 0.000350 | 0.011630 |
| Glycitein 7-O-glucuronide | 0.9481 | 0.9508 | 0.000564 | 0.000358 |
| 3-Hexenedioic acid | 0.8988 | 0.8835 | 0.000468 | 0.000373 |
| Quercetin 3-beta-D-glucoside | 0.1667 | 0.3477 | 0.000221 | 0.003706 |
| Suillusin | 0.9085 | 0.8765 | 0.025080 | 0.003962 |
| Quercitrin | 0.3424 | 0.4269 | 0.005149 | 0.019290 |
| 2-(2,4,5-trihydroxyphenyl)propanoic acid | 0.8598 | 0.8242 | 0.000018 | 0.000004 |
| Gallic acid | 0.8407 | 0.8203 | 0.000139 | 0.000259 |
| Hydroxynalidixic acid | 0.7424 | 0.5703 | 0.001262 | 0.000037 |
| Monoisobutyl phthalic acid | 0.8310 | 0.8122 | 0.038310 | 0.024760 |
| Aphidicolin | 1.0361 | 0.9679 | 0.047610 | 0.002636 |
| (S)-Nerolidol 3-O-[a-L-rhamnopyranosyl-(1->2)-b-D-glucopyranoside] | 4.0915 | 4.3595 | 0.012820 | 0.014030 |
| 2-trans,4-cis-Decadienoylcarnitine | 1.5375 | 1.5394 | 0.009313 | 0.014230 |
| 1400W | 1.0851 | 1.1047 | 0.023520 | 0.002727 |
| S-Adenosylhomocysteine | 1.1778 | 1.2802 | 0.014540 | 0.019620 |
| Tragopogonsaponin A | 1.1101 | 1.1266 | 0.010460 | 0.003836 |